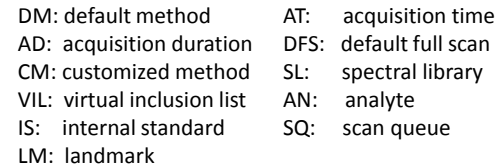


Flow process chart of the IS-PRM application



Installation of the application

Pre-requirements

The access to API functionality will be provided by Thermo Fisher Scientific. The license is available upon request and acceptance of terms and conditions. The application has been developed in C# programming language. Microsoft .NET framework 4 is required to install the application.

Procedure

The compressed folder “IS-PRM” downloaded from **Supplementary Material** (Snapshot 1) needs to be uncompressed on the computer that controls the mass spectrometer (Snapshot 2). The uncompressed folder contains several components necessary to the installation and two .csv files to be used as templates to prepare the acquisition method and the spectral library (Snapshot 3). The installation of the application is started by clicking “setup.exe” (Snapshot 4) and then the button “Install” in the security warning message (Snapshot 5). At the end of the installation the interface of the application is displayed (Snapshot 6).

Execution of the application

Procedure

The application is started automatically following the installation, as described above, or by clicking the application icon accessible *via* the start menu (Snapshot 7). Then the upload of the necessary information to the application is carried out *via* the file menu (Snapshot 8). First, the spectral library is selected (Snapshots 9, 10, and 11). Second, the file defining the acquisition parameters of the IS-PRM method can be defined by clicking the “Import Customized Method” command. However, at the time of the first use of the application, the command may remain inaccessible (in grey, Snapshot 12). Closing and restarting the application (Snapshot 7) fix the issue (Snapshot 13) and allow the selection of the IS-PRM method file (Snapshot 13, 14, 15, and 16). Third, the selection of the default method (allowing the definition of the acquisition duration of the analysis and the parameters to be used to acquire the first full MS spectra during the acquisition) is performed (Snapshot 17, 18, and 19). Fourth, the raw file number and its associated location path are defined *via* the “Options” command in the “Tools” menu (Snapshot 20 and 21). Fifth, all the defined information is pre-uploaded by clicking the “Preload” command in the “Tools” menu (Snapshot 22). The absence of error messages appearing in a separated window and in the main window of the interface (Snapshot 23) confirms that the spectral library and method files were prepared in an appropriate format and that a reference MS/MS spectrum is present in the spectral library for each of the internal standard peptides included in the IS-PRM method. Sixth, the actual upload of the information to the acquisition software is performed by clicking the “Connect” button (Snapshot 24). The main window of the interface indicates the proper connection to the instrument (Snapshot 25), which means that the instrument is ready to receive the contact closure

signal from the chromatographic system and to start the acquisition. Last, the chromatographic analysis is started (see “Tips” section below) and triggers by a contact closure signal the start of the MS acquisition (Snapshot 26).

Requirements

The spectral library is prepared in .csv format. A template for the spectral library is provided in the uncompressed folder of **Supplementary Material** (Snapshot 3). The formatting of the file is displayed in Snapshot 27 for a couple of peptides (two internal standard and one landmark peptides). Briefly, columns A and B indicate the peptide sequence and the precursor m/z. In column C, the m/z of the fragment ions to be used in the spectral matching are indicated while their associated intensities are reported in column F. For the internal standards (peptides GNFHAVYR and FYNIGDQR in the example), the columns D and E define the initial monitoring window (RT start and stop), while this information is used to defined the reference elution time of the landmark peptides (center value of the window, *i.e.*, 15.81 min for the peptide SSAAPPPPPR in the example). The chromatographic peak width and the minimum intensity threshold are defined in the columns G and H, respectively. For landmark peptides, the chromatographic peak width is set to 0 as the monitoring window of these peptides is not modified during IS-PRM analysis.

The definition of the acquisition parameters of the IS-PRM method is included in a .csv file (“Customized method”). A template is provided in the uncompressed folder of **Supplementary Material** (Snapshot 3). The formatting of the file is displayed in Snapshot 28 for a series of peptides (seven pairs of SIL and endogenous peptides and thirteen landmark peptides). This file indicates the acquisition parameters to be used for the PRM measurement of the internal standards in “watch mode” (term “Standard” in column H), the PRM measurement of the internal standards and the analytes in “quantitative mode” (term “Analyte” in column H), and the PRM measurement of the landmark peptides (term “Landmark” in column H). The acquisition parameters include the m/z of the center value of the quadrupole isolation window used for the isolation of the peptide ions (column B), the corresponding charge state (column C) which is used to define the m/z range of the MS/MS spectra and the collision energy (in conjunction with the normalized collision energy value indicated in column L), the width of the quadrupole isolation window (column E), the orbitrap resolving power (Column K), and the AGC target value (Column M). The settings of the monitoring windows are only indicated (and not modified during the acquisition) for landmark peptides as those of the internal standards are defined in the spectral library (initial values which are modified following the detection of the landmark peptides and/or their own detection) while those of the analytes are defined based on the detection of their corresponding internal standard. Each pair of SIL and endogenous peptides is defined by a common term in column I, which is the sequence of the SIL peptide used as internal standard in the

example. The acquisition parameters to perform the full scan acquisition are also indicated in the file (line 36 in the example defining an m/z 300-1500 mass selection).


Comments and tips

- The settings of the tolerances to be used for real-time spectral matching are accessible *via* the “Options” command in the “Tools” menu (Snapshots 20 and 21). The precursor ion tolerance parameter (in ppm) defines the tolerance to be used for the comparison of the center value of the quadrupole isolation window employed to generate a given MS/MS spectrum and the precursor m/z value of the internal standards, as defined in the spectral library. The fragment ion tolerance parameters defines the tolerance (in ppm) used for the extraction of the signals of the fragment ions (defined in the spectral library).
- The sequences and m/z values of the internal standards in column A of the two .csv files needs to be in full agreement for proper operation of the acquisition.
- The order used to include the PRM scans of internal standards, analytes, and landmark peptides, and the full scan in the “customized method” file needs to be maintained for proper acquisition.
- The internal standards are included two times and designated once by the term “Standard” and once by the term “Analyte” in column H in the “Customized method” file. This is to distinguish the acquisition parameters to be used in the “watch mode” and in the “quantitative mode”.
- The default method is prepared with the standard method editor (Snapshot 29) and only includes a full scan event that should be designed with the same acquisition parameters settings as those used to define the full scan in the “customized method” file to maintain consistency.
- With the current version of the application, the mass spectrometer needs to be removed from the instrument configuration in Thermo foundation if the chromatographic system is controlled by Xcalibur. Alternatively, the chromatographic system can be controlled with a separated computer and/or program. Also, no batch mode is available with the current version of the application. The analyses need to be started one by one while restarting the application before each new run.
- The application has been tested successfully using Thermo Foundation 3.0 (build number 138), Thermo Xcalibur 3.0 (build number 63), and Thermo Exactive Series 2.3 (build 1765). It has also been briefly tested using Thermo Foundation 3.0 SP2 (build number 152), Thermo Xcalibur 3.0 (build number 63), and Thermo Exactive Series 2.4 (build 1824).
- Punctually, the acquisition starts immediately after clicking the “Connect” button (Snapshot 24) and before receiving the contact closure signal from the chromatographic system. In this case, the acquisition needs to be stopped (*via* the tune interface) and the application closed and restarted.
- Acquisition freezes occasionally for IS-PRM methods including a very large number of targets. This requires to restart the electronics of the mass spectrometer. Avoiding manual stop of the acquisition

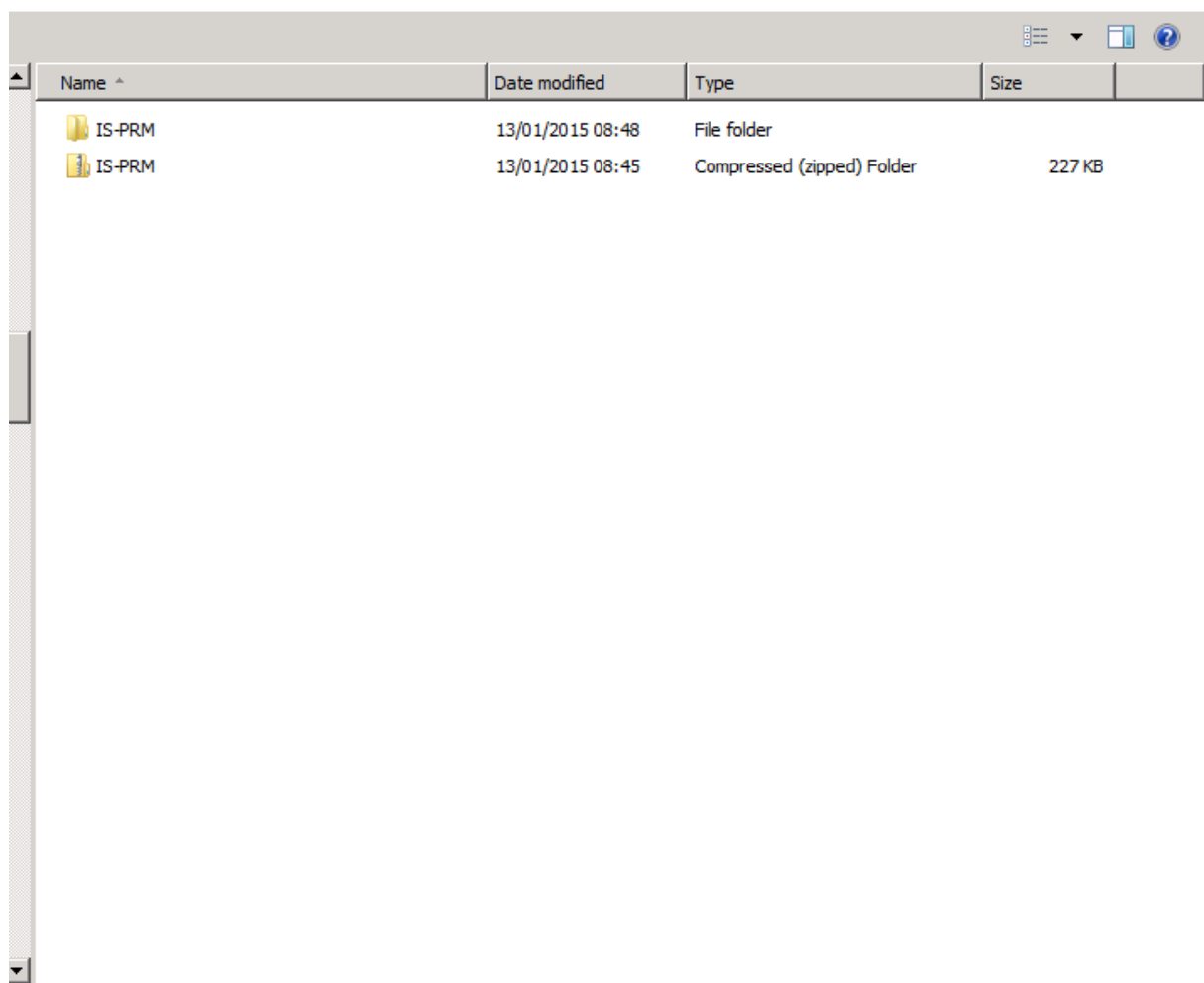
(by pressing the “stop” button in the Tune interface) and closing other programs with high demand in resources alleviate the issue.

- At the end of the acquisition, a log file (.txt format) capturing all pertinent information of the analysis (e.g., the detection of the internal standards, the detection of landmark peptides, etc...) is created (Snapshot 30).



Snapshot 1

Name ^	Date modified	Type	Size
 IS-PRM	13/01/2015 08:45	Compressed (zipped) Folder	227 KB

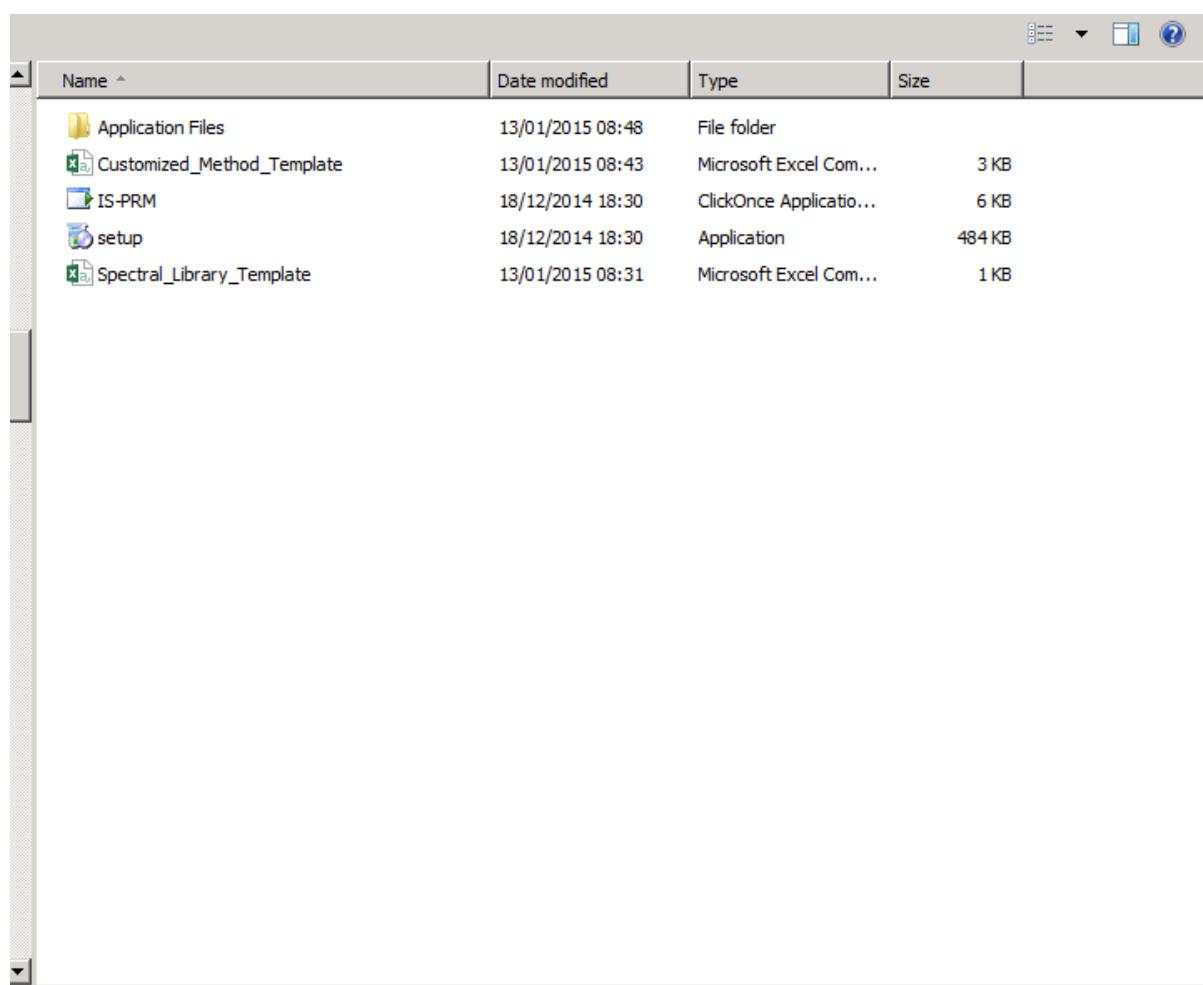
Snapshot 2








The image shows a screenshot of a file explorer window. The window has a title bar with standard icons (minimize, maximize, close) and a help icon. Below the title bar is a toolbar with icons for view (list, icons, details), a dropdown arrow, a refresh icon, and a help icon. The main area displays a table of files and folders. The table has five columns: Name, Date modified, Type, Size, and an empty column. There are two rows of data. The first row shows a folder named 'IS-PRM' with a date modified of '13/01/2015 08:48', type 'File folder', and size '227 KB'. The second row shows a compressed folder named 'IS-PRM' with a date modified of '13/01/2015 08:45', type 'Compressed (zipped) Folder', and size '227 KB'. The window has a vertical scrollbar on the left side.

Name ^	Date modified	Type	Size	
 IS-PRM	13/01/2015 08:48	File folder		
 IS-PRM	13/01/2015 08:45	Compressed (zipped) Folder	227 KB	

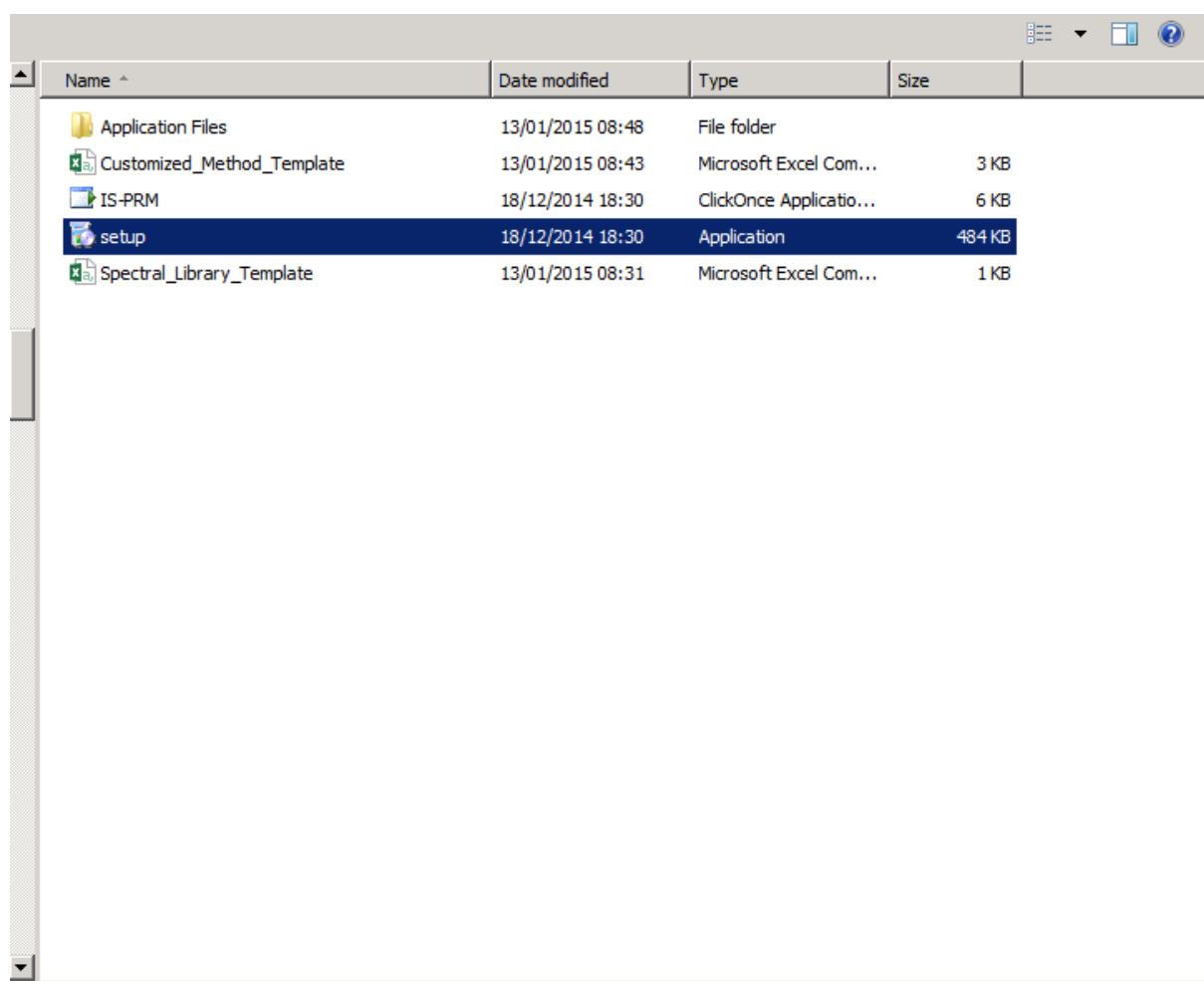
Snapshot 3



The image shows a screenshot of a file explorer window. The window has a title bar with standard icons (minimize, maximize, close) and a help icon. Below the title bar is a toolbar with icons for view (list, icons, web view), a dropdown arrow, a new folder icon, and a help icon. The main area displays a table of files and folders. The table has five columns: Name, Date modified, Type, Size, and an empty column. The files listed are: Application Files (File folder), Customized_Method_Template (Microsoft Excel Com...), IS-PRM (ClickOnce Applicatio...), setup (Application), and Spectral_Library_Template (Microsoft Excel Com...). The file 'setup' is highlighted.

Name ^	Date modified	Type	Size	
 Application Files	13/01/2015 08:48	File folder		
 Customized_Method_Template	13/01/2015 08:43	Microsoft Excel Com...	3 KB	
 IS-PRM	18/12/2014 18:30	ClickOnce Applicatio...	6 KB	
 setup	18/12/2014 18:30	Application	484 KB	
 Spectral_Library_Template	13/01/2015 08:31	Microsoft Excel Com...	1 KB	

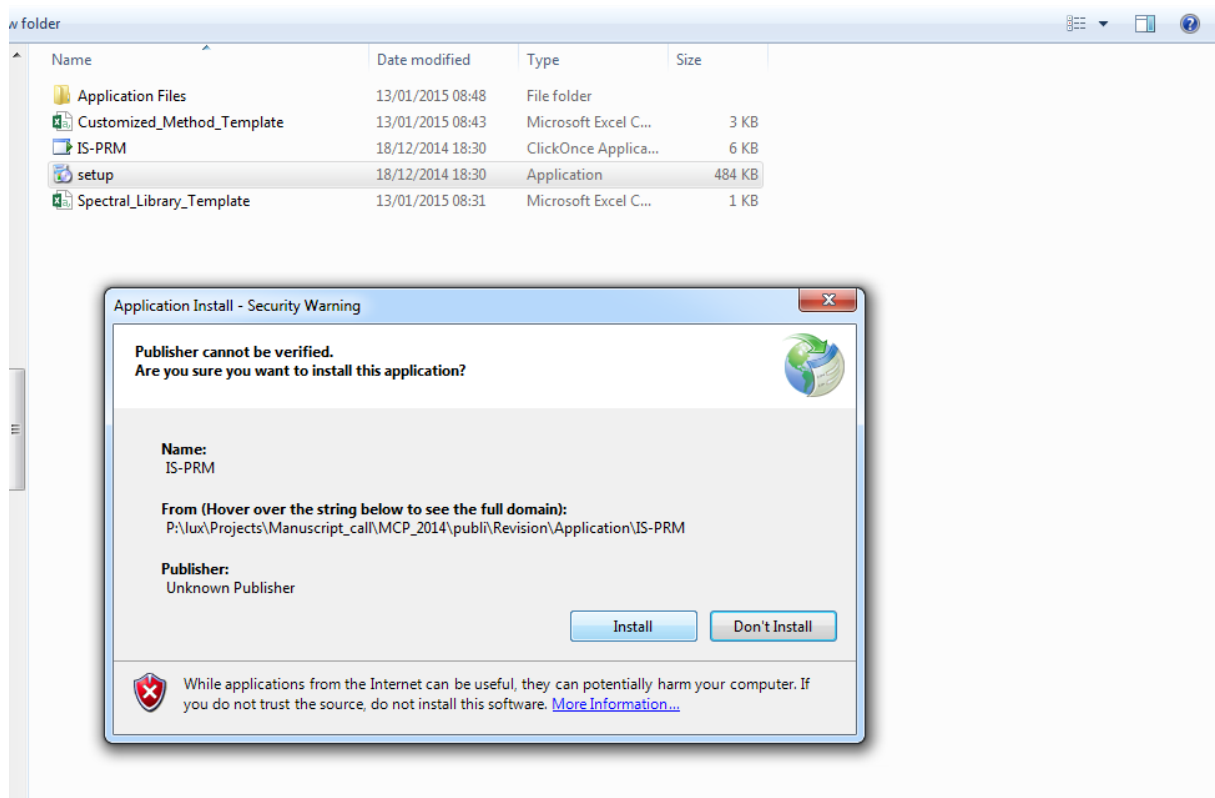
Snapshot 4



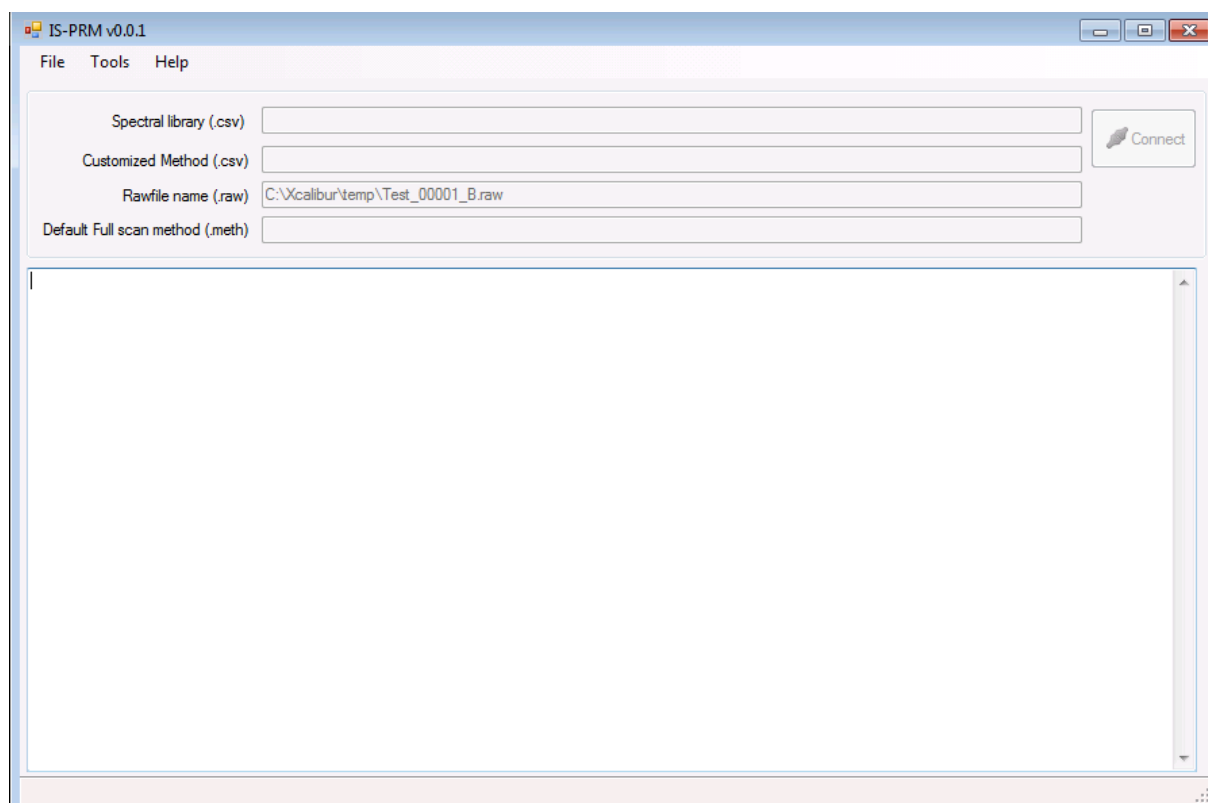
A screenshot of a Windows Explorer window. The window title bar is not visible. The address bar is empty. The main pane shows a list of files and folders. The 'setup' file is selected, highlighted in blue. The file list has columns for Name, Date modified, Type, and Size. The 'setup' file is an Application, 484 KB, modified on 18/12/2014 18:30. Other files include 'Application Files' (Folder), 'Customized_Method_Template' (Excel Com..., 3 KB), 'IS-PRM' (ClickOnce Applicatio..., 6 KB), and 'Spectral_Library_Template' (Excel Com..., 1 KB).

Name	Date modified	Type	Size
Application Files	13/01/2015 08:48	File folder	
Customized_Method_Template	13/01/2015 08:43	Microsoft Excel Com...	3 KB
IS-PRM	18/12/2014 18:30	ClickOnce Applicatio...	6 KB
setup	18/12/2014 18:30	Application	484 KB
Spectral_Library_Template	13/01/2015 08:31	Microsoft Excel Com...	1 KB

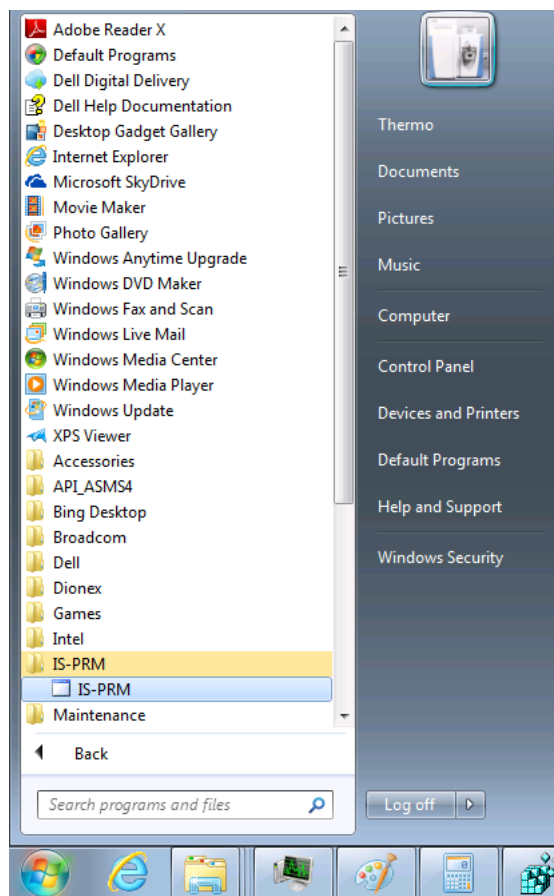
Snapshot 5



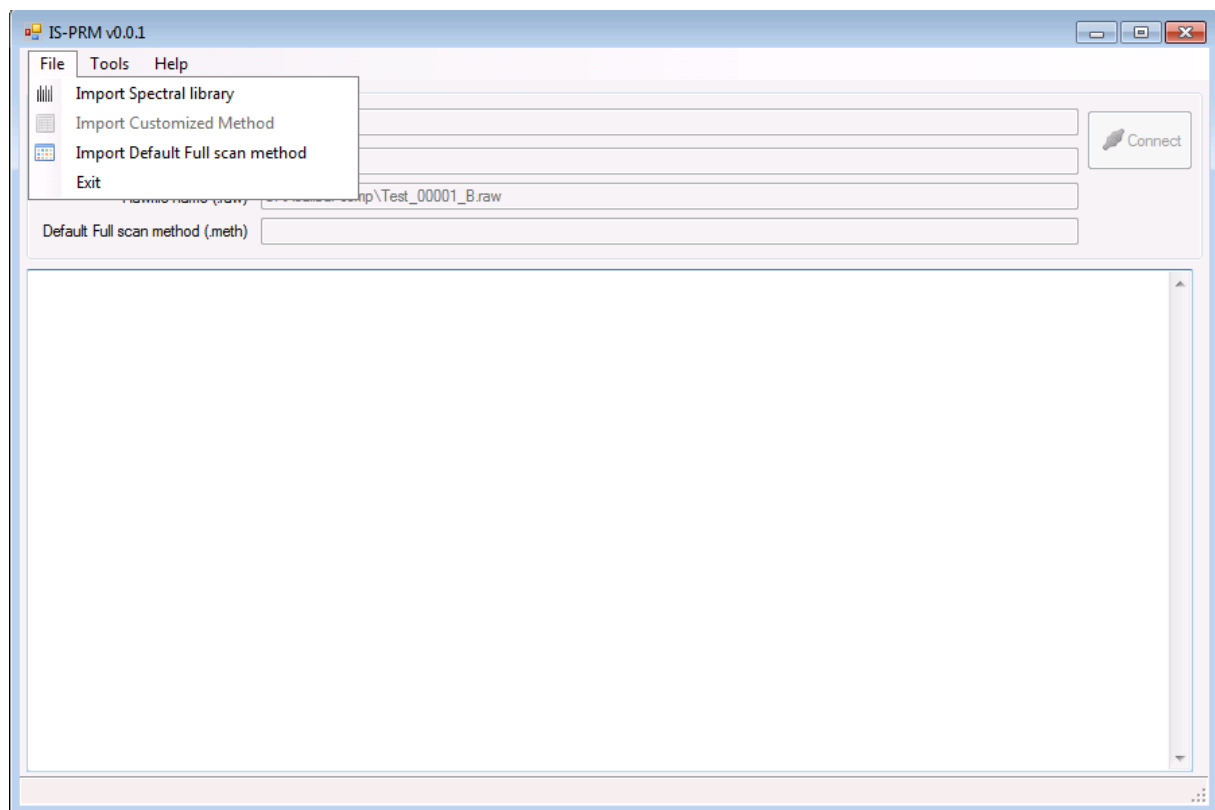
Snapshot 6



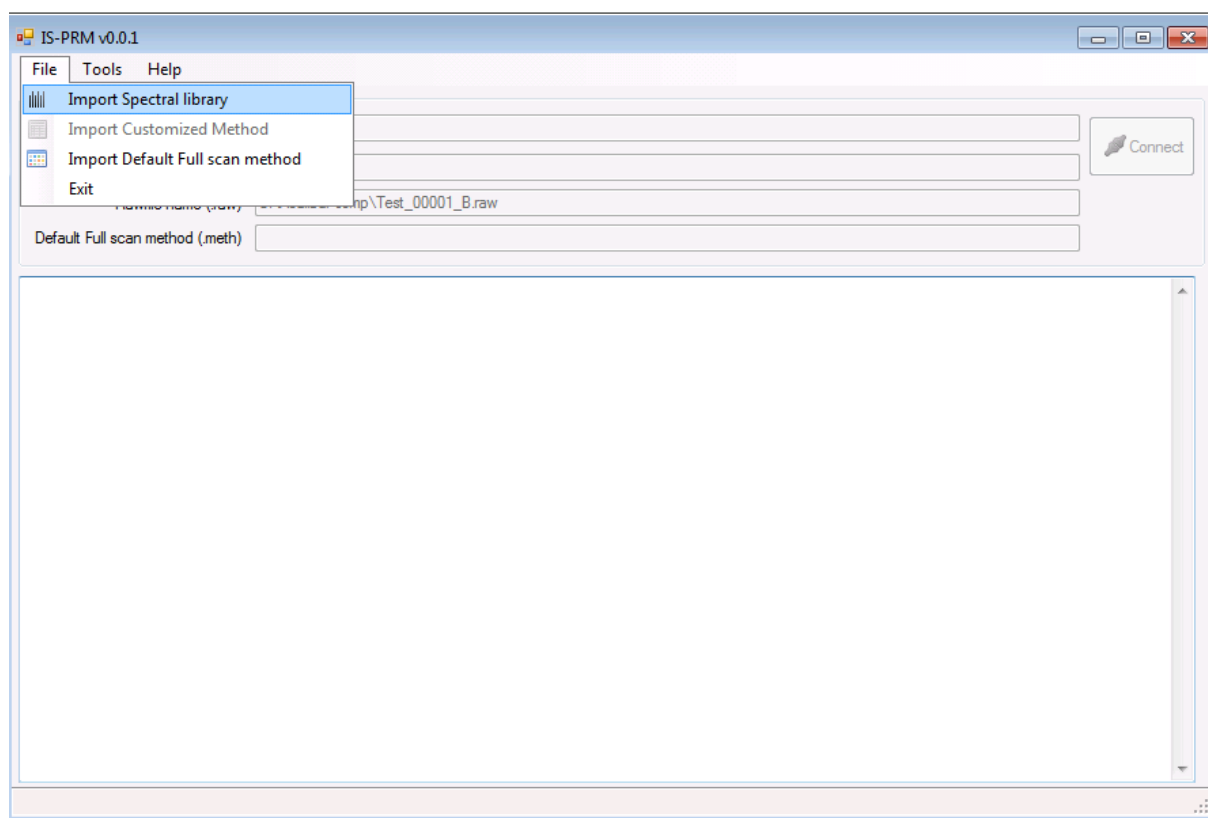
Snapshot 7



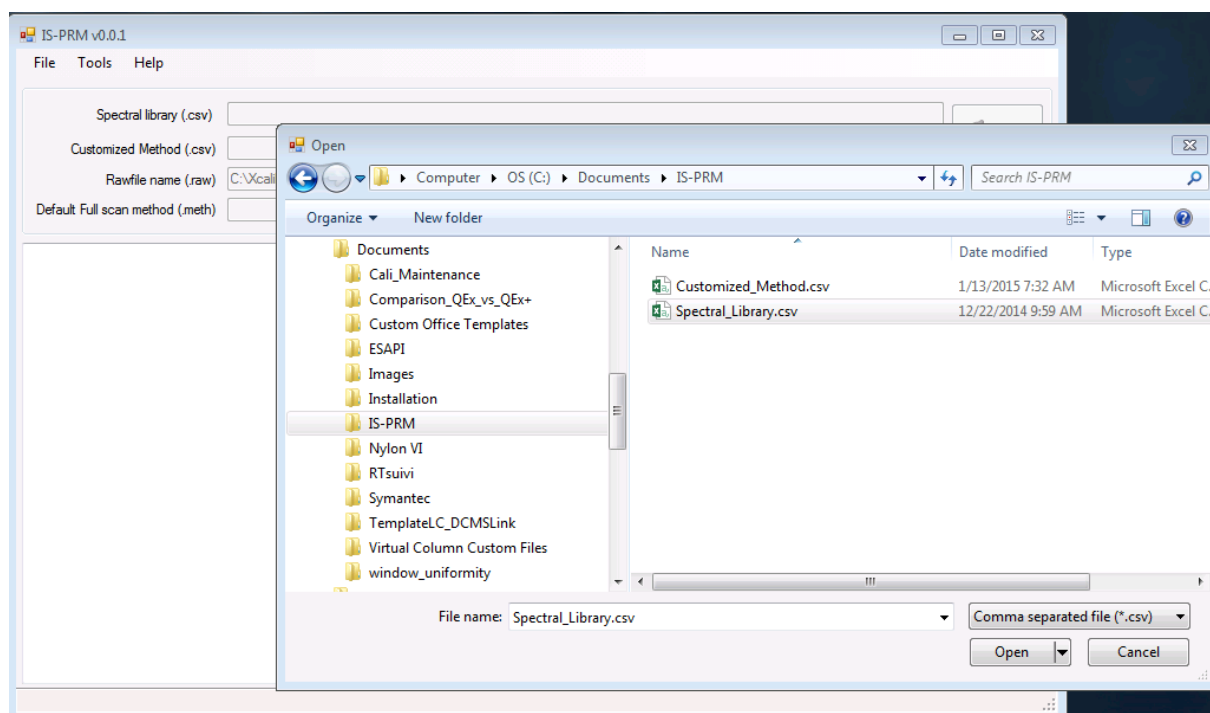
Snapshot 8



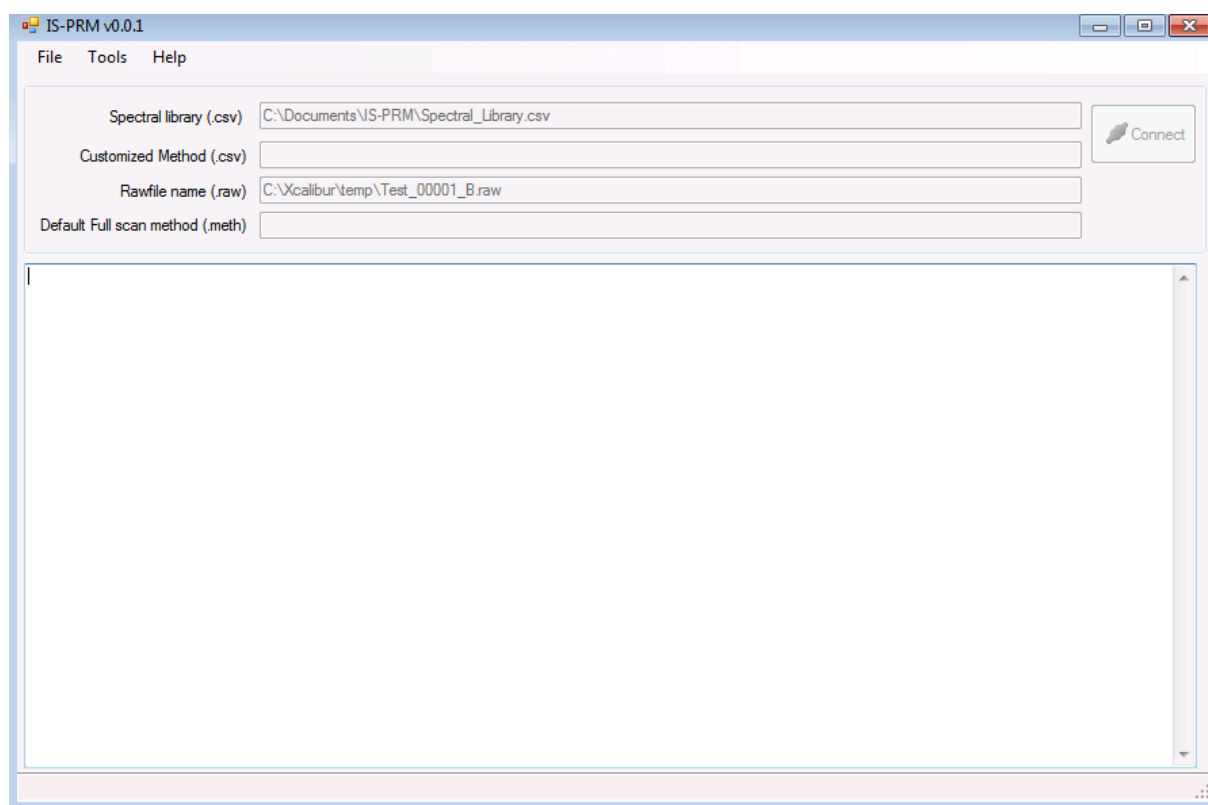
Snapshot 9



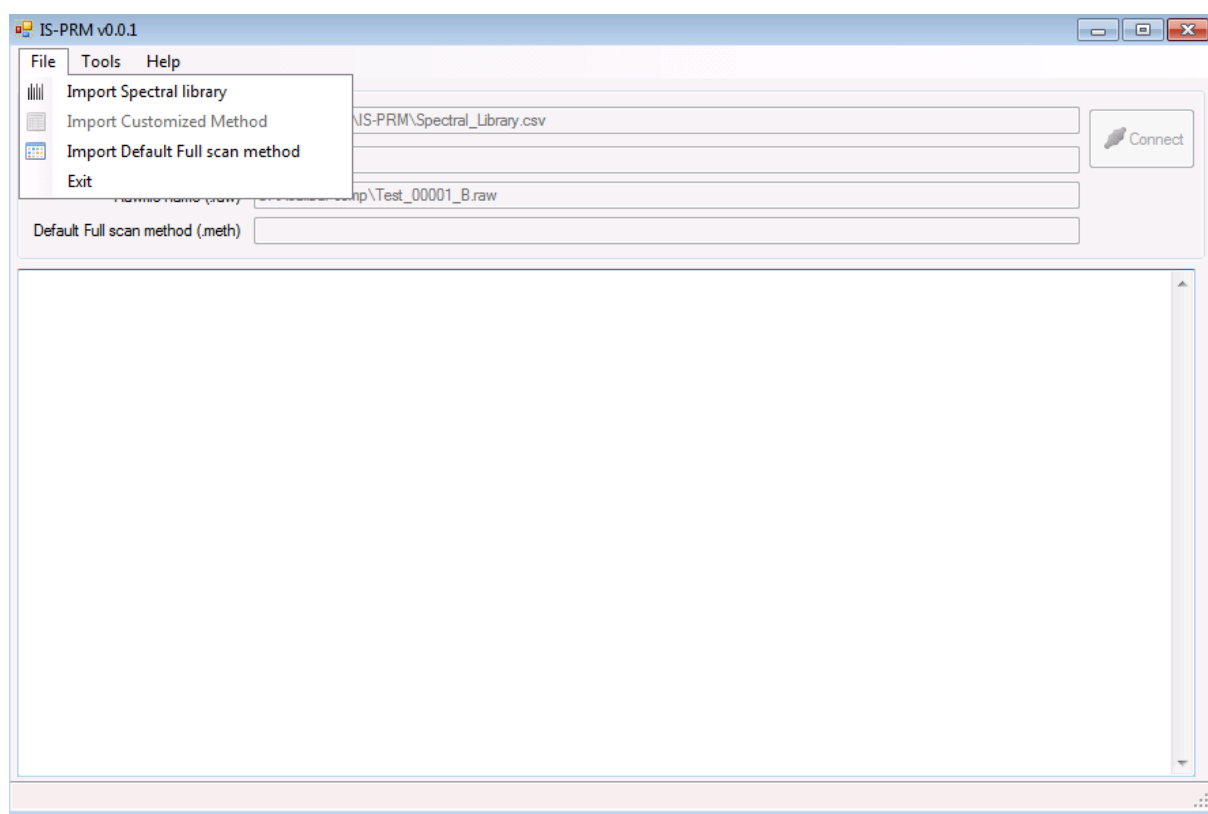
Snapshot 10



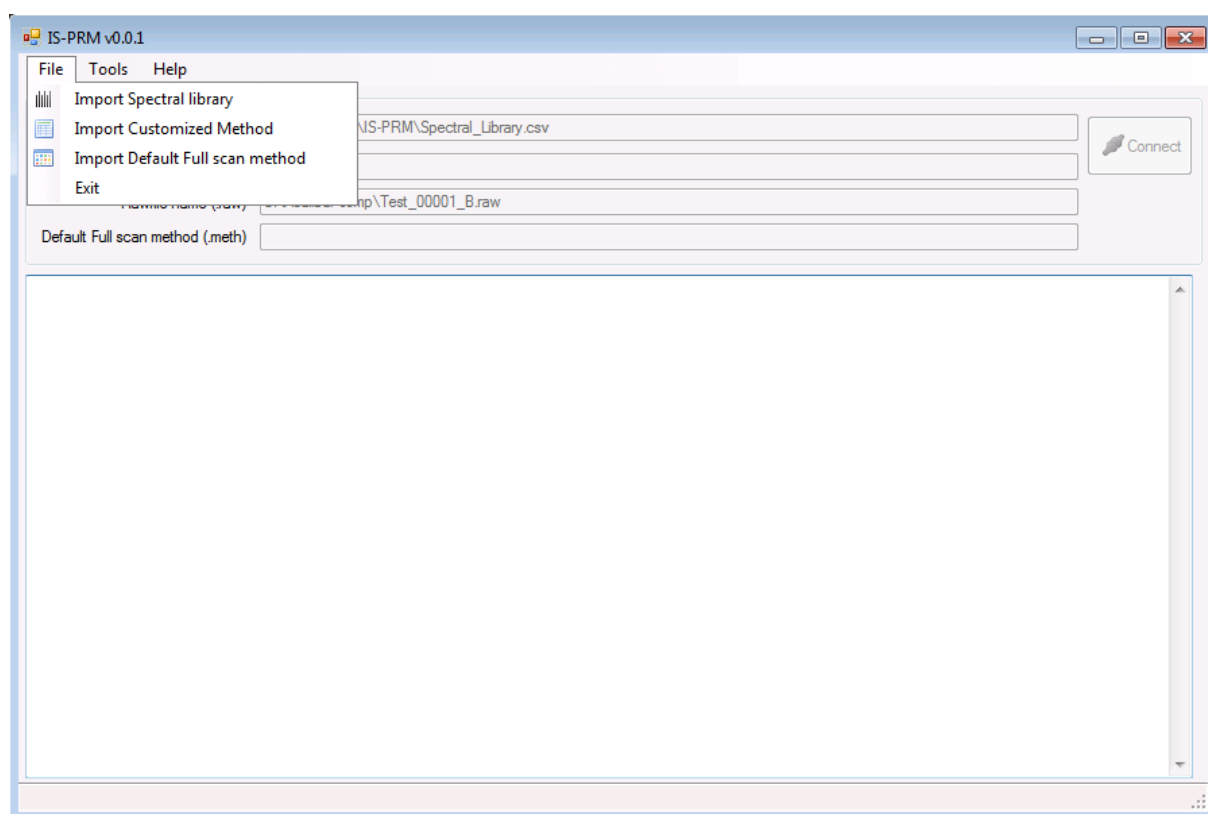
Snapshot 11



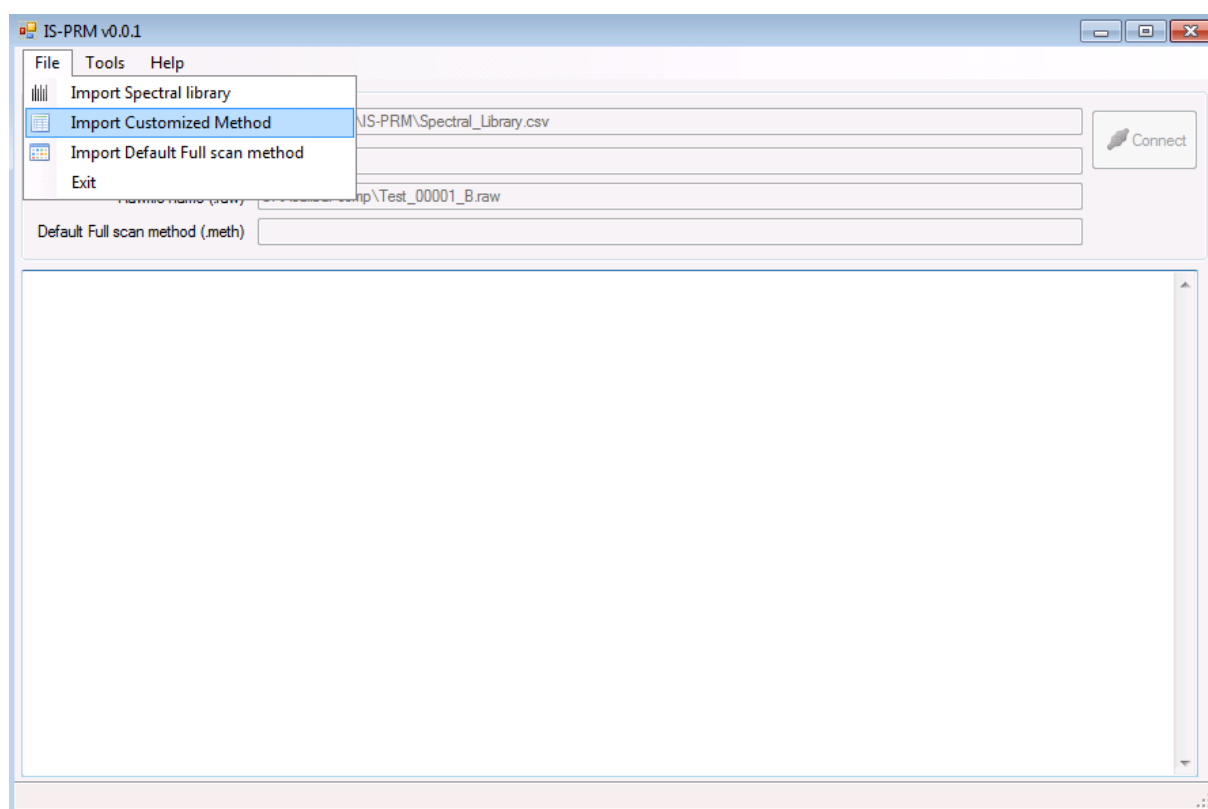
Snapshot 12



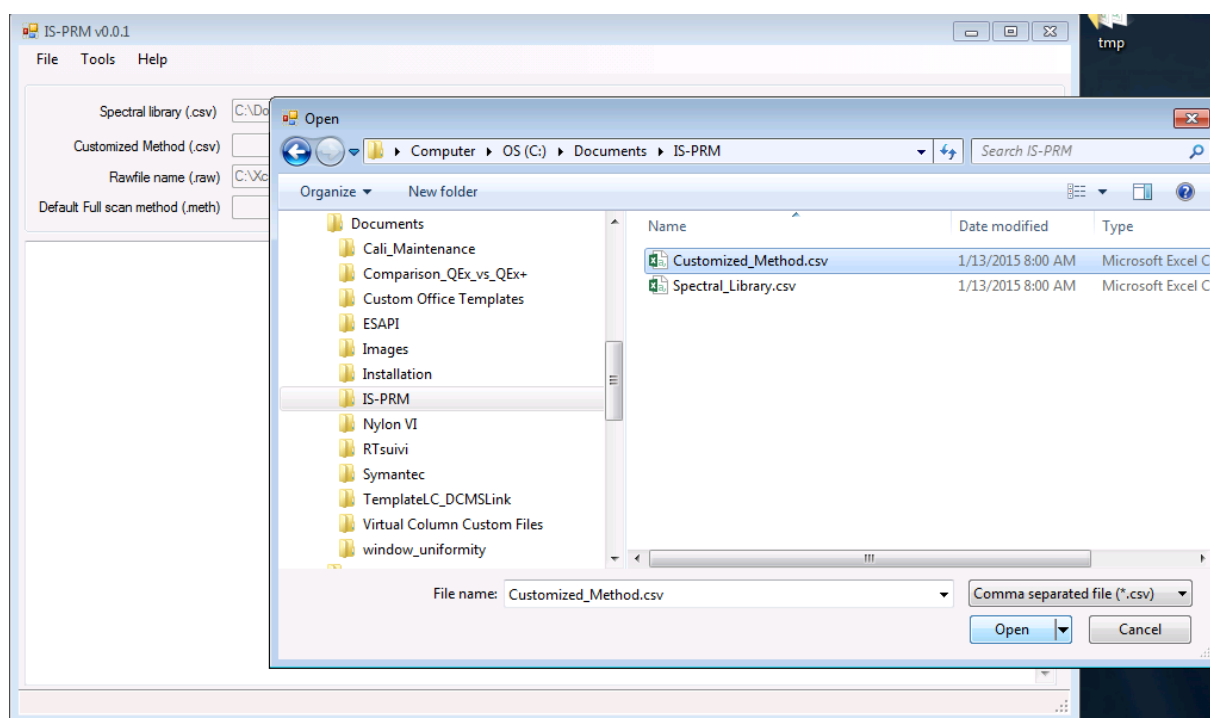
Snapshot 13



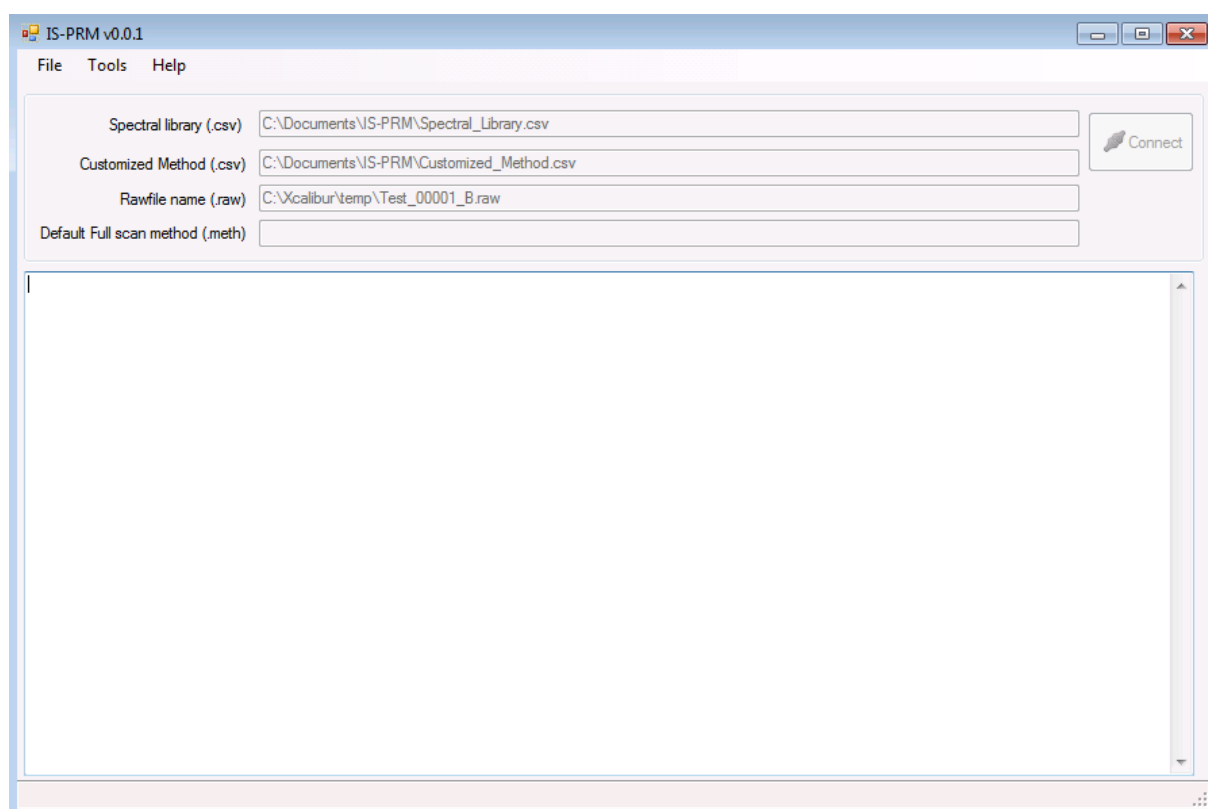
Snapshot 14



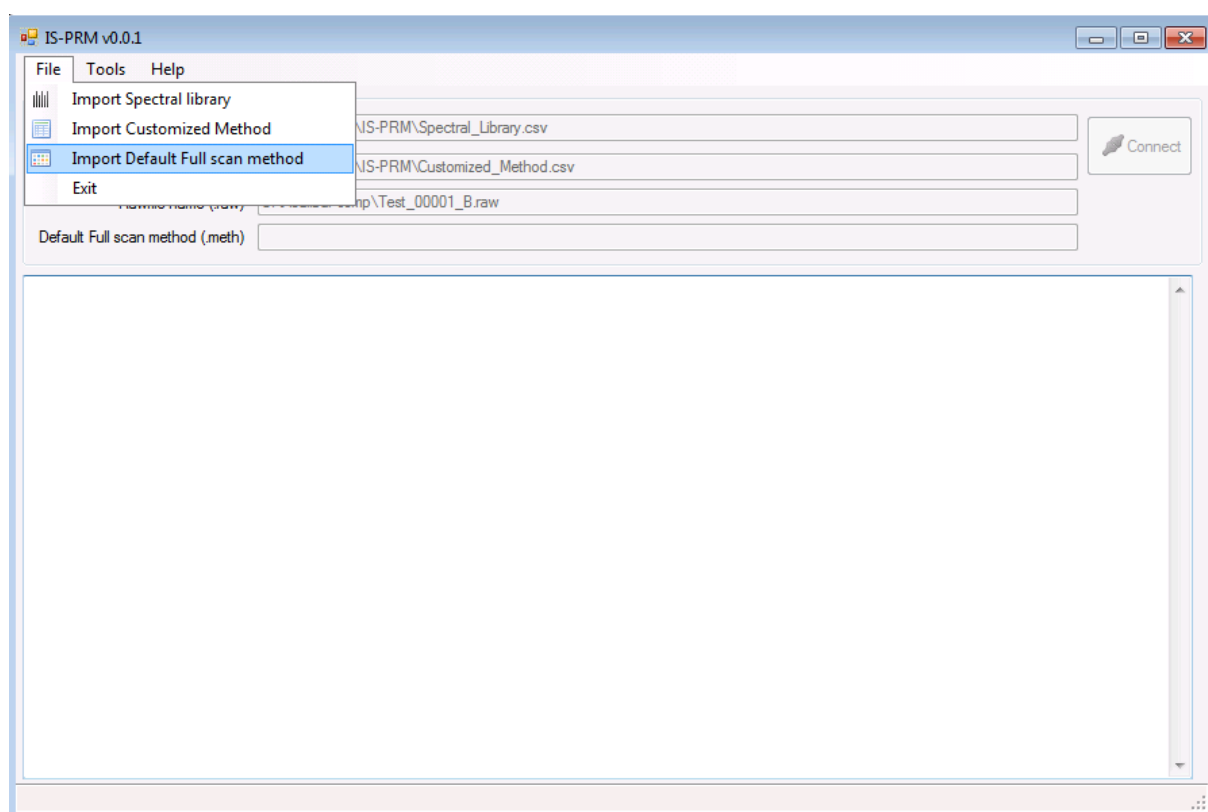
Snapshot 15



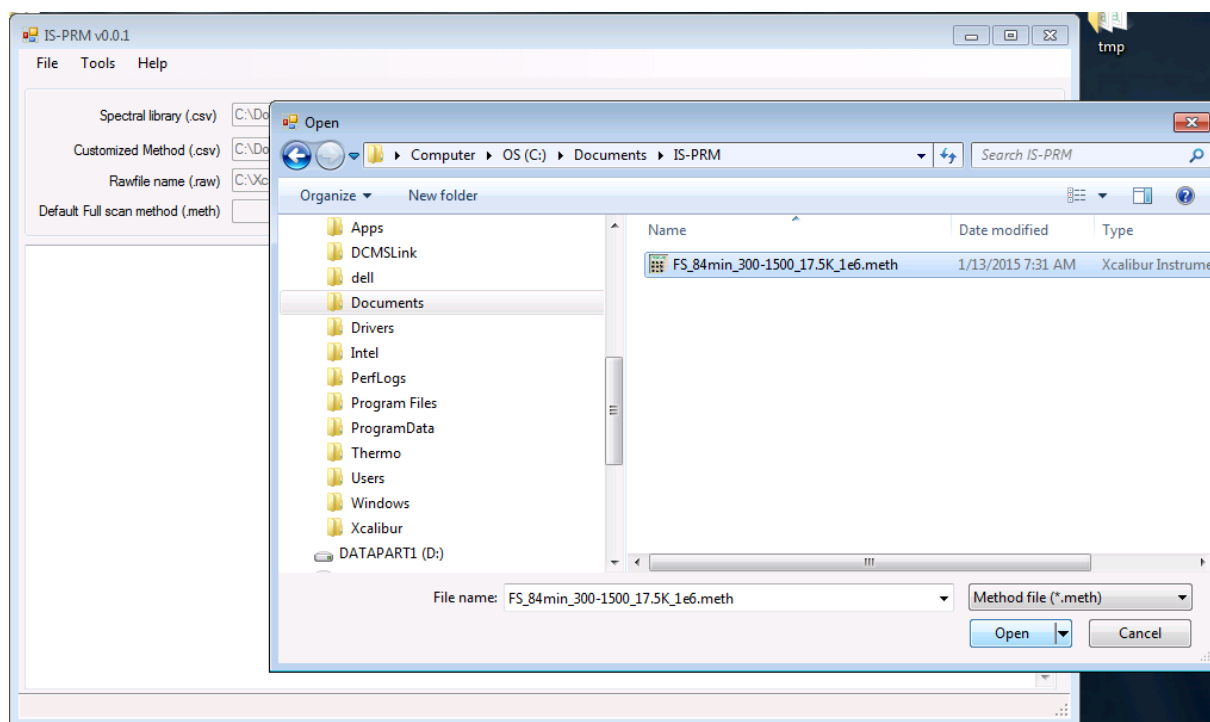
Snapshot 16



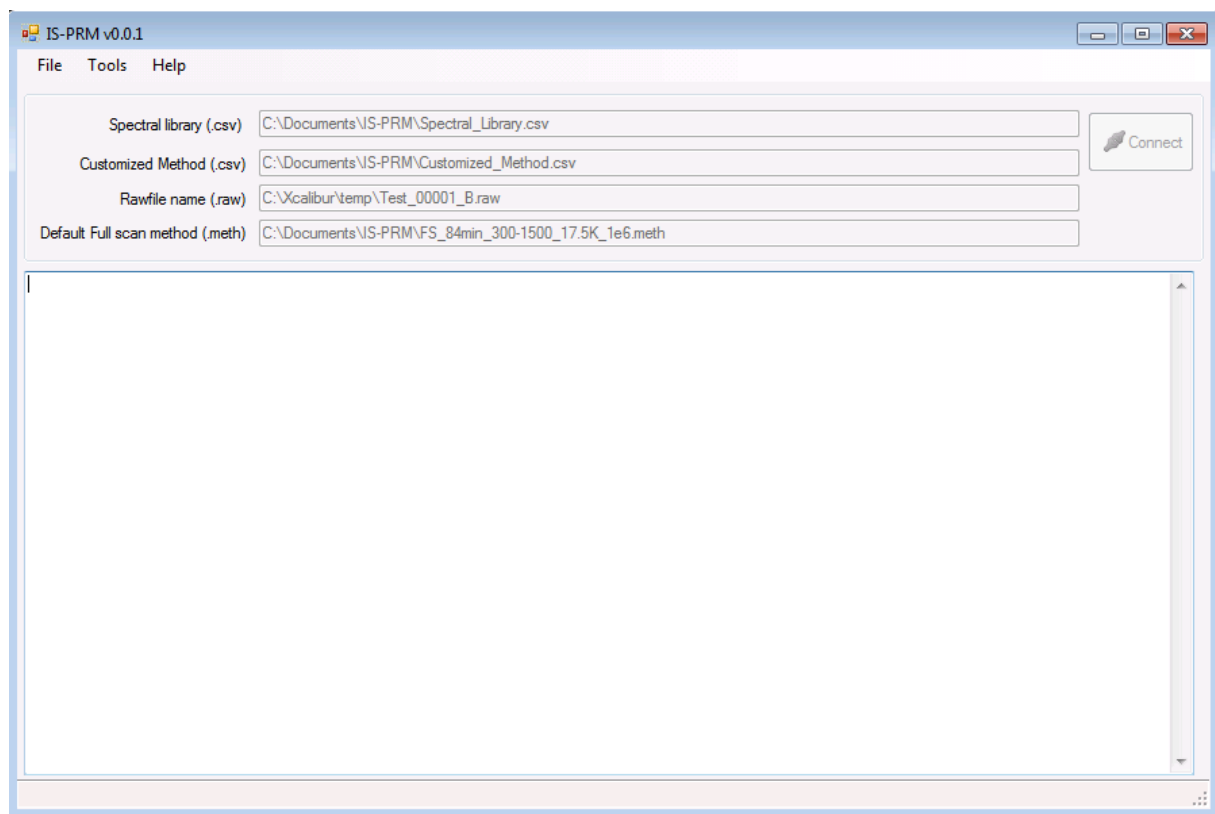
Snapshot 17



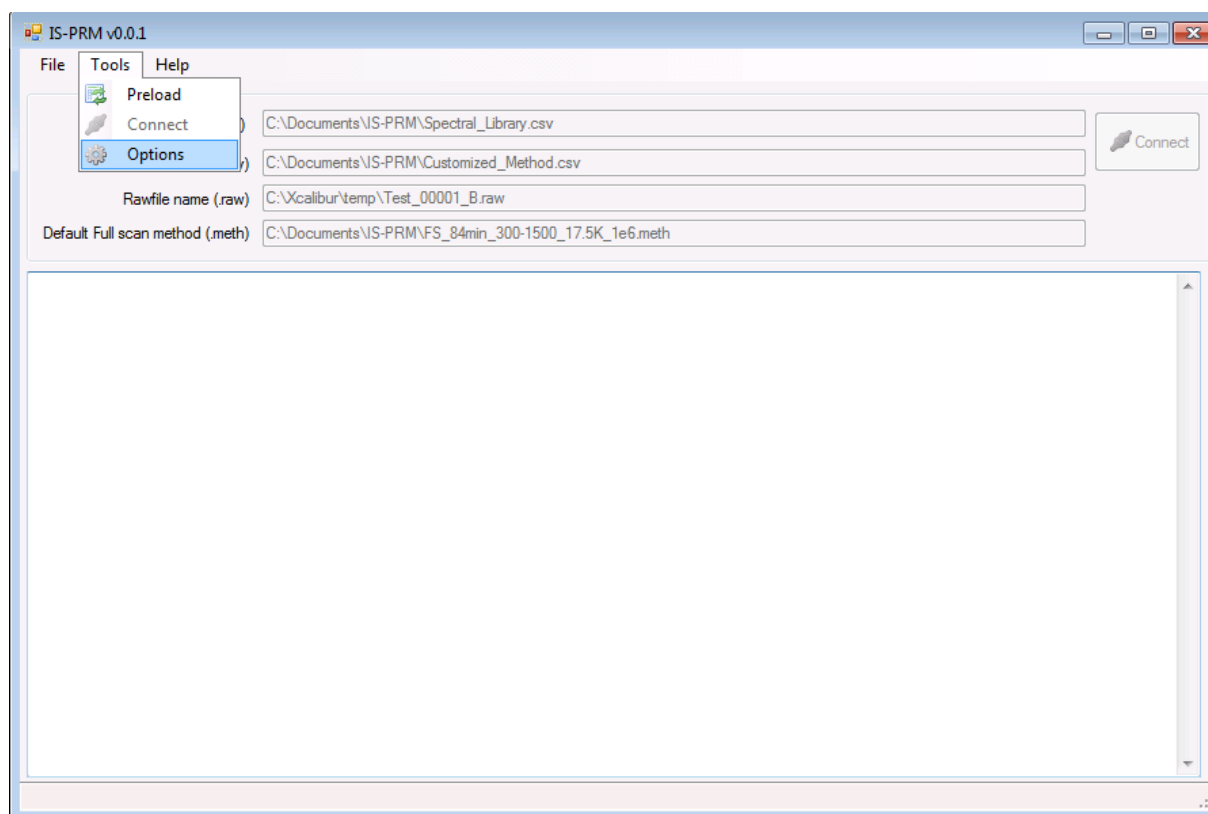
Snapshot 18



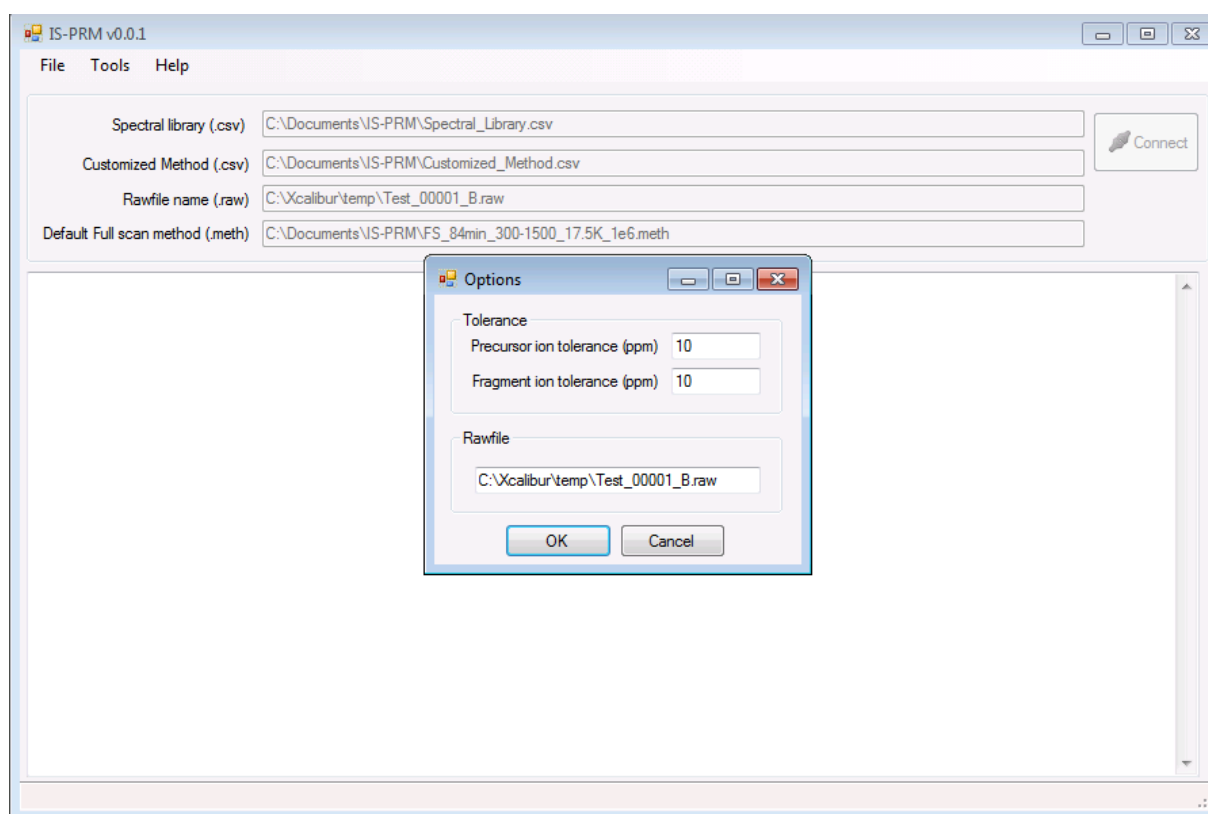
Snapshot 19



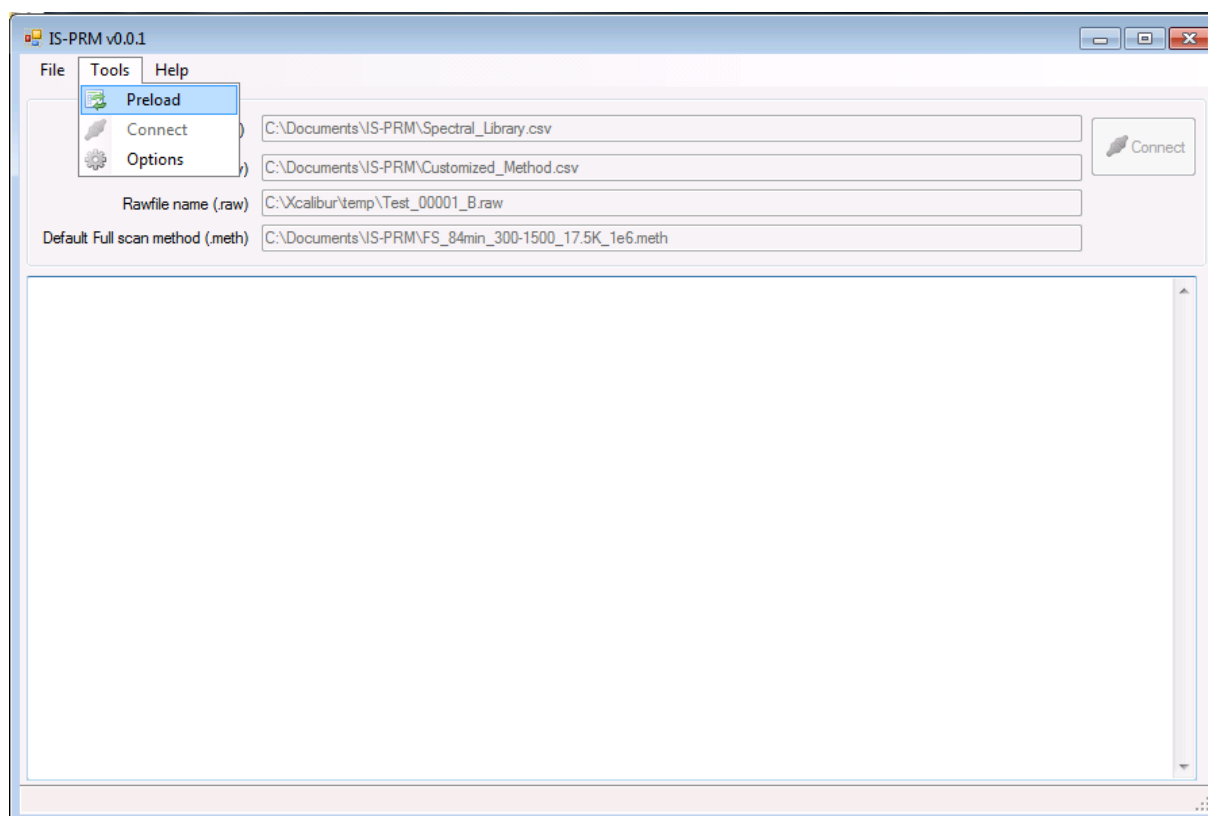
Snapshot 20



Snapshot 21



Snapshot 22



Snapshot 23

IS-PRM v0.0.1

File Tools Help

Spectral library (.csv) C:\Documents\IS-PRM\Spectral_Library.csv

Customized Method (.csv) C:\Documents\IS-PRM\Customized_Method.csv

Rawfile name (.raw) C:\Xcalibur\temp\Test_00001_B.raw

Default Full scan method (.meth) C:\Documents\IS-PRM\FS_84min_300-1500_17.5K_1e6.meth

Connect

#[13 Jan 08:22:01] SpectLib table: C:\Documents\IS-PRM\Customized_Method.csv
 #[13 Jan 08:22:01] Loaded 619 reference Spectra.

HVFGQPVK[HEAVYK]	460.266	[6]	14	35055	0.5
FESSEEQAR[HEAVYR]	546.745	[6]	14	284600	0.5
NIIHGSDSVK[HEAVYK]	539.293	[6]	14	89700	0.5
FGSDDEGR[HEAVYR]	446.687	[6]	14	356400	0.5
AFDSGDGR[HEAVYR]	475.198	[6]	14	480650	0.5
GQNSLALHK[HEAVYK]	488.277	[6]	14	294550	0.5
GLQTSQDAR[HEAVYR]	493.25	[6]	14	424700	0.5
APAVAEENPK[HEAVYK]	517.274	[6]	14	392450	0.5
TTTPNAQATR[HEAVYR]	535.777	[6]	14	367450	0.5
LADGGATNQGR[HEAVYR]	535.267	[6]	14	222750	0.5
AASQPGELK[HEAVYK]	454.75	[6]	14	1512500	0.5
ATVNPSAPR[HEAVYR]	461.753	[6]	14	1450000	1
NANAEPVQR[HEAVYR]	540.277	[6]	14	386750	0.5
LVEGESDNR[HEAVYR]	514.748	[6]	14	552500	0.5
LASAYGAR[HEAVYR]	409.723	[6]	14	368150	0.5
YAEAVTR[HEAVYR]	410.215	[6]	14	361100	0.5
GPPASSPAPK[HEAVYK]	542.797	[6]	14	351600	0.5
SSAAPPPPPR[HEAVYR]	493.768	[6]	15.81	1000000	0
FAHTVVTSR[HEAVYR]	514.282	[6]	16.319	1015500	0.5
DADDPPTYGNSAK[HEAVYK]	631.275	[6]	16.732	669500	0.5
SDHPAILR[HEAVYR]	459.755	[6]	16.977	772000	0.5
AVTEQGHLSNEER[HEAVYR]	804.878	[6]	17.008	5055	0.5
LTWASHEK[HEAVYK]	490.258	[6]	17.1	294550	0.5
GNFHAVYR[HEAVYR]	487.248	[6]	17.197	12180	0.5
ATEHLSTLSEK[HEAVYK]	612.322	[6]	17.268	831500	0.5
QIDNPDK[HEAVYK]	500.745	[6]	17.535	39965	0.5

Snapshot 24

IS-PRM v0.0.1

File Tools Help

Spectral library (.csv) C:\Documents\IS-PRM\Spectral_Library.csv

Customized Method (.csv) C:\Documents\IS-PRM\Customized_Method.csv

Rawfile name (.raw) C:\Xcalibur\temp\Test_00001_B.raw

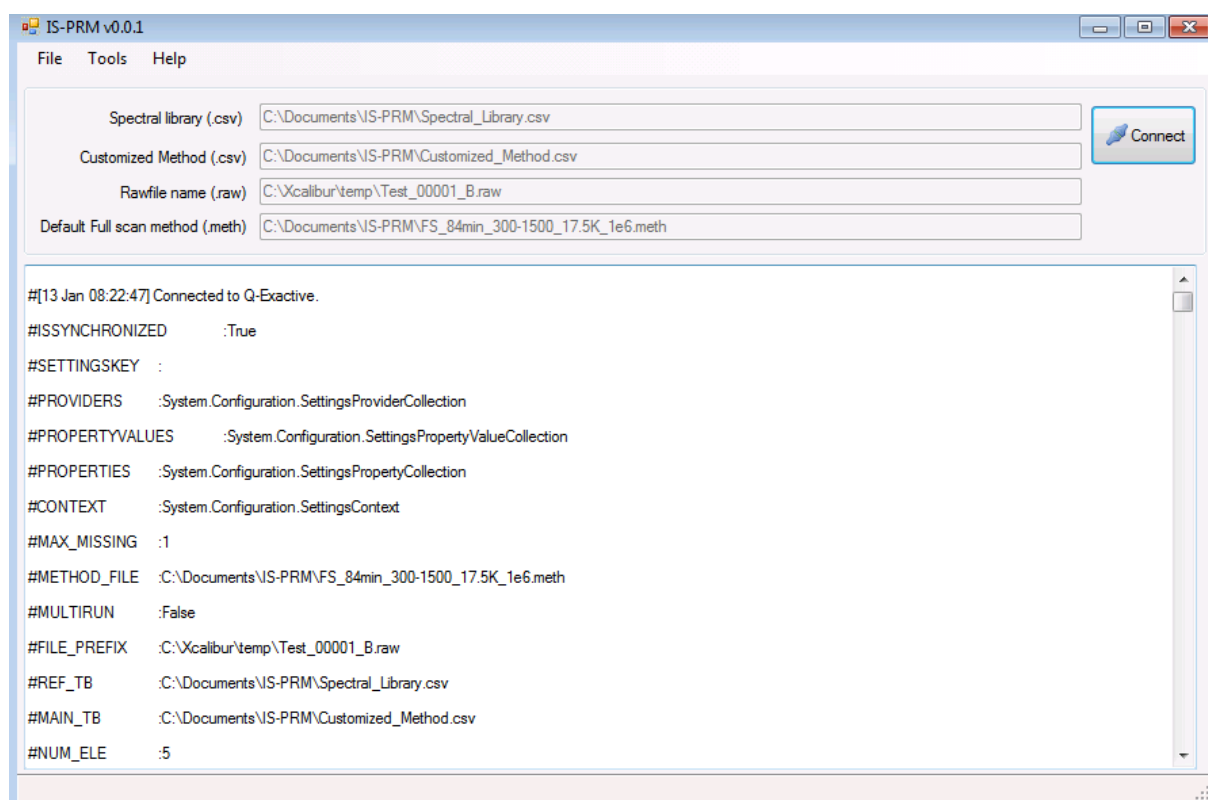
Default Full scan method (.meth) C:\Documents\IS-PRM\FS_84min_300-1500_17.5K_1e6.meth

Connect

#[13 Jan 08:22:01] SpectLib table: C:\Documents\IS-PRM\Customized_Method.csv
#[13 Jan 08:22:01] Loaded 619 reference Spectra.

HVFGQPVK[HEAVYK]	460.266	[6]	14	35055	0.5
FESSEEQAR[HEAVYR]	546.745	[6]	14	284600	0.5
NIHGSQSVK[HEAVYK]	539.293	[6]	14	89700	0.5
FGSDDEGR[HEAVYR]	446.687	[6]	14	356400	0.5
AFDSDGDGR[HEAVYR]	475.198	[6]	14	480650	0.5
GQNSLALHK[HEAVYK]	488.277	[6]	14	294550	0.5
GLQTSQDAR[HEAVYR]	493.25	[6]	14	424700	0.5
APAVAEENPK[HEAVYK]	517.274	[6]	14	392450	0.5
TTTTNAQATR[HEAVYR]	535.777	[6]	14	367450	0.5
LADGGATNQGR[HEAVYR]	535.267	[6]	14	222750	0.5
AASQPGELK[HEAVYK]	454.75	[6]	14	1512500	0.5
ATVNPAPR[HEAVYR]	461.753	[6]	14	1450000	1
NANAEPVQR[HEAVYR]	540.277	[6]	14	386750	0.5
LVEGESDNR[HEAVYR]	514.748	[6]	14	552500	0.5
LASAYGAR[HEAVYR]	409.723	[6]	14	368150	0.5
YAEAVTR[HEAVYR]	410.215	[6]	14	361100	0.5
GPPASSPAPAK[HEAVYK]	542.797	[6]	14	351600	0.5
SSAAPPPPPR[HEAVYR]	493.768	[6]	15.81	1000000	0
FAHTVTSR[HEAVYR]	514.282	[6]	16.319	1015500	0.5
DADDPTYGNSAK[HEAVYK]	631.275	[6]	16.732	669500	0.5
SDHPAILR[HEAVYR]	459.755	[6]	16.977	772000	0.5
AVTEGGHELSNEER[HEAVYR]	804.878	[6]	17.008	5055	0.5
LTWASHEK[HEAVYK]	490.258	[6]	17.1	294550	0.5
GNFHAVYR[HEAVYR]	487.248	[6]	17.197	12180	0.5
ATEHLSTLSEK[HEAVYK]	612.322	[6]	17.268	831500	0.5
QIDNPDK[HEAVYK]	500.745	[6]	17.535	39965	0.5

Snapshot 25



Snapshot 26

IS-PRM v0.0.1

File Tools Help

Spectral library (.csv) C:\Documents\IS-PRM\Spectral_Library.csv

Customized Method (.csv) C:\Documents\IS-PRM\Customized_Method.csv

Rawfile name (.raw) C:\Xcalibur\temp\Test_00001_B.raw

Default Full scan method (.meth) C:\Documents\IS-PRM\FS_84min_300-1500_17.5K_1e6.meth

Connect

#[13 Jan 08:26:44] Acquisition Started!
 #[13 Jan 08:26:43] Contact Closure started
 #[13 Jan 08:26:43] Trigger Contact Closure

#[13 Jan 08:22:01] SpectLib table: C:\Documents\IS-PRM\Customized_Method.csv
 #[13 Jan 08:22:01] Loaded 619 reference Spectra.

HVFGQPVK[HEAVYK]	460.266	[6]	14	35055	0.5
FESSEEQAR[HEAVYR]	546.745	[6]	14	284600	0.5
NIIHGSDSVK[HEAVYK]	539.293	[6]	14	89700	0.5
FGSDDEGR[HEAVYR]	446.687	[6]	14	356400	0.5
AFDSDGDGR[HEAVYR]	475.198	[6]	14	480650	0.5
GQNSLALHK[HEAVYK]	488.277	[6]	14	294550	0.5
GLQTSQDAR[HEAVYR]	493.25	[6]	14	424700	0.5
APAVAEENPK[HEAVYK]	517.274	[6]	14	392450	0.5
TTTTNAQATR[HEAVYR]	535.777	[6]	14	367450	0.5
LADGGATNQGR[HEAVYR]	535.267	[6]	14	222750	0.5
AASQPGELK[HEAVYK]	454.75	[6]	14	1512500	0.5
ATVNPAPPR[HEAVYR]	461.753	[6]	14	1450000	1
NANAEPVQR[HEAVYR]	540.277	[6]	14	386750	0.5
LVEGESDNR[HEAVYR]	514.748	[6]	14	552500	0.5
LASAYGAR[HEAVYR]	409.723	[6]	14	368150	0.5
YAEAVTR[HEAVYR]	410.215	[6]	14	361100	0.5
GPPASSPAPAK[HEAVYK]	542.797	[6]	14	351600	0.5
SSAAPPPPPR[HEAVYR]	493.768	[6]	15.81	1000000	0
FAHTVVTSR[HEAVYR]	514.282	[6]	16.319	1015500	0.5
DADDPPTYGNSAK[HEAVYK]	631.275	[6]	16.732	669500	0.5
SDHPAILR[HEAVYR]	459.755	[6]	16.977	772000	0.5
AVTEQGHLSNEER[HEAVYR]	804.878	[6]	17.008	5055	0.5

Snapshot 27

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1	GNFHAVYR[HeavyR]			16.696816	17.696816		0.5	12180														
2		487.248																				
3			518.2955			2469000																
4			328.1808			1344000																
5			655.3544			1285000																
6			447.2584			628200																
7			401.7151			307300																
8			802.4229			294900																
9	FYNIGDQR[HeavyR]			26.360653	27.360653		0.5	60100														
10		511.75																				
11			712.3607			1.73E+07																
12			485.2336			9.44E+06																
13			598.3177			5.70E+06																
14			875.424			3.29E+06																
15			428.2122			7.04E+05																
16			313.1852			2.50E+07																
17	SSAAPPPPR[HeavyR]			15.31	16.31		0	1000000														
18		493.768																				
19			379.2322			5.49E+06																
20			476.285			3.21E+07																
21			573.3377			3.56E+07																
22			670.3905			8.40E+07																
23			246.1079			2.47E+07																
24			317.145			8.89E+06																
25																						
26																						
27																						
28																						
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34																						
35																						

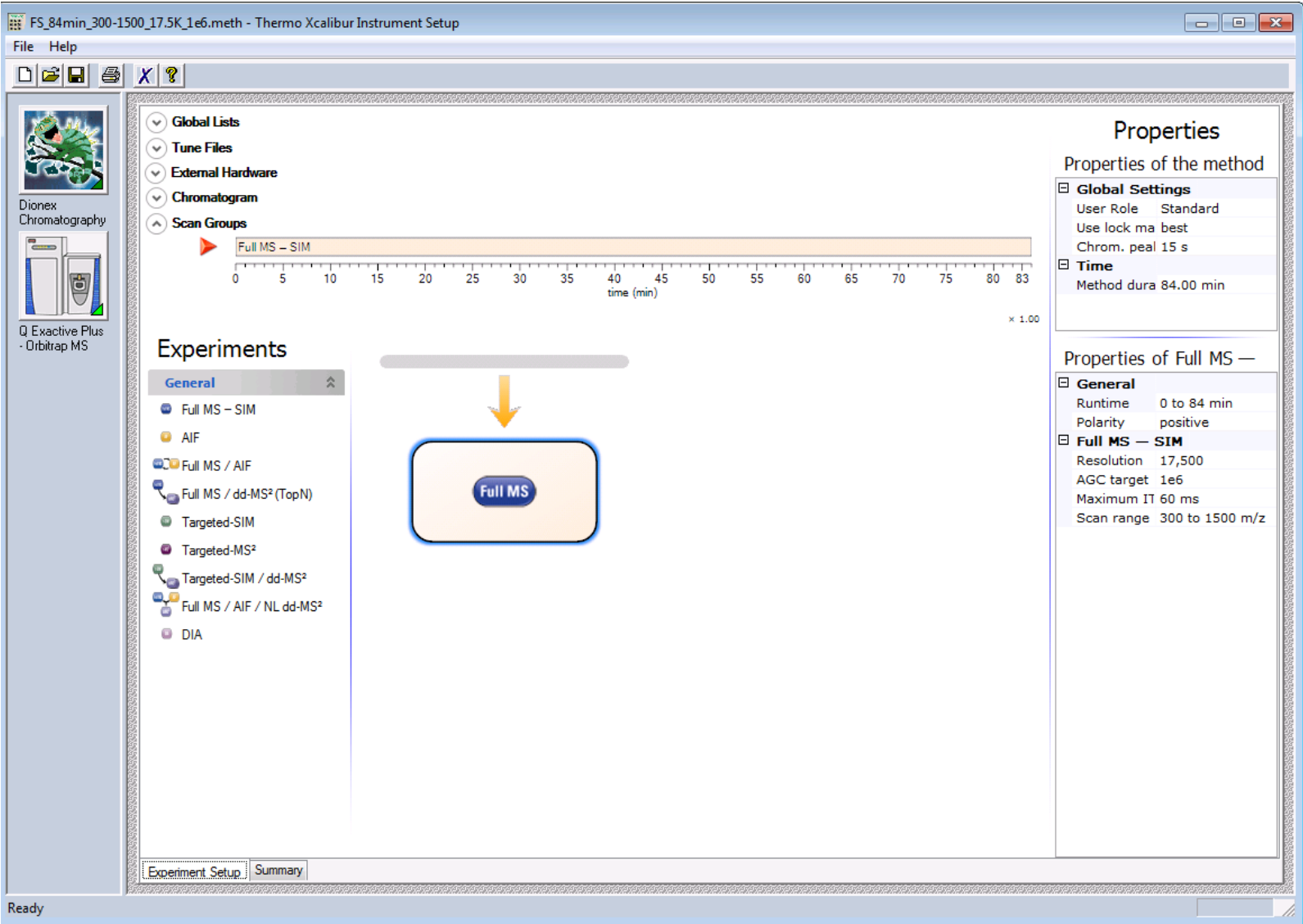
Spectral_Library_Template

Snapshot 28

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
	Peptide	m/z	Charge_State	Scan_Type	Isolation window	RT start	RT stop	Designation_iPRM	Group iPRM	MaxIT	Resolution	NCE	AGC_Target		
1	GNFHAVYR[HeavyR]	487.248	2	PRM	2			Standard	GNFHAVYR[HeavyR]	20	15000	25	1000000		
2	FYNIGDQR[HeavyR]	511.75	2	PRM	2			Standard	FYNIGDQR[HeavyR]	20	15000	25	1000000		
3	LAQAAQSSVATITR[HeavyR]	713.898	2	PRM	2			Standard	LAQAAQSSVATITR[HeavyR]	20	15000	25	1000000		
4	IYVVDVGSEPR[HeavyR]	622.331	2	PRM	2			Standard	IYVVDVGSEPR[HeavyR]	20	15000	25	1000000		
5	GVALADFNR[HeavyR]	486.76	2	PRM	2			Standard	GVALADFNR[HeavyR]	20	15000	25	1000000		
6	GSAPPGVPVEGSIR[HeavyR]	665.853	2	PRM	2			Standard	GSAPPGVPVEGSIR[HeavyR]	20	15000	25	1000000		
7	IAYGTQGSSGYSLR[HeavyR]	735.367	2	PRM	2			Standard	IAYGTQGSSGYSLR[HeavyR]	20	15000	25	1000000		
8	GNFHAVYR[HeavyR]	487.248	2	PRM	2			Analyte	GNFHAVYR[HeavyR]	20	15000	25	1000000		
9	FYNIGDQR[HeavyR]	511.75	2	PRM	2			Analyte	FYNIGDQR[HeavyR]	20	15000	25	1000000		
10	LAQAAQSSVATITR[HeavyR]	713.898	2	PRM	2			Analyte	LAQAAQSSVATITR[HeavyR]	20	15000	25	1000000		
11	IYVVDVGSEPR[HeavyR]	622.331	2	PRM	2			Analyte	IYVVDVGSEPR[HeavyR]	20	15000	25	1000000		
12	GVALADFNR[HeavyR]	486.76	2	PRM	2			Analyte	GVALADFNR[HeavyR]	20	15000	25	1000000		
13	GSAPPGVPVEGSIR[HeavyR]	665.853	2	PRM	2			Analyte	GSAPPGVPVEGSIR[HeavyR]	20	15000	25	1000000		
14	IAYGTQGSSGYSLR[HeavyR]	735.367	2	PRM	2			Analyte	IAYGTQGSSGYSLR[HeavyR]	20	15000	25	1000000		
15	GNFHAVYR	482.2434	2	PRM	2			Analyte	GNFHAVYR[HeavyR]	110	60000	25	1000000		
16	FYNIGDQR	506.7459	2	PRM	2			Analyte	FYNIGDQR[HeavyR]	110	60000	25	1000000		
17	LAQAAQSSVATITR	708.8938	2	PRM	2			Analyte	LAQAAQSSVATITR[HeavyR]	110	60000	25	1000000		
18	IYVVDVGSEPR	617.3273	2	PRM	2			Analyte	IYVVDVGSEPR[HeavyR]	110	60000	25	1000000		
19	GVALADFNR	481.7563	2	PRM	2			Analyte	GVALADFNR[HeavyR]	110	60000	25	1000000		
20	GSAPPGVPVEGSIR	660.8489	2	PRM	2			Analyte	GSAPPGVPVEGSIR[HeavyR]	110	60000	25	1000000		
21	IAYGTQGSSGYSLR	730.3624	2	PRM	2			Analyte	IAYGTQGSSGYSLR[HeavyR]	110	60000	25	1000000		
22	SSAAPPPPR[HeavyR]	493.768	2	PRM	2	5	19	Landmark		60	17500	25	1000000		
23	GISNEGQNASIK[HeavyK]	613.317	2	PRM	2	5	21	Landmark		60	17500	25	1000000		
24	DIPVPKPK[HeavyK]	451.283	2	PRM	2	5	25	Landmark		60	17500	25	1000000		
25	IGDYAGIK[HeavyK]	422.7363	2	PRM	2	19	26	Landmark		60	17500	25	1000000		
26	TASEFDSAIAQDK[HeavyK]	695.832	2	PRM	2	21	31	Landmark		60	17500	25	1000000		
27	SAAGAFGPESLR[HeavyR]	586.8003	2	PRM	2	25	33	Landmark		60	17500	25	1000000		
28	ELGQSGVDTYLQTK[HeavyK]	773.8955	2	PRM	2	26	37	Landmark		60	17500	25	1000000		
29	GLILVGGYGTR[HeavyR]	558.3259	2	PRM	2	31	40	Landmark		60	17500	25	1000000		
30	SFANQPLEVVYSK[HeavyK]	745.3924	2	PRM	2	33	42	Landmark		60	17500	25	1000000		
31	LTILEELR[HeavyR]	498.8018	2	PRM	2	37	45	Landmark		60	17500	25	1000000		
32	NGFILDGFPR[HeavyR]	573.3025	2	PRM	2	40	70	Landmark		60	17500	25	1000000		
33	ELASGLSFPVGFK[HeavyK]	680.3735	2	PRM	2	42	70	Landmark		60	17500	25	1000000		
34	LSSEAPALFQFDLK[HeavyK]	787.4212	2	PRM	2	45	70	Landmark		60	17500	25	1000000		
35		900		FS		1200	0	84		60	17500		1000000		
36															
37															

Customized_Method_Template

Snapshot 29



Snapshot 30

File	Edit	Format	View	Help
SN#:21749,	RT(min):28.117864,	IsCustom:False,	left_num_queue:12,	Candidates:46 , Type:System.Boolean, #of Candies:1832
SN#:21750,	RT(min):28.120205,	IsCustom:False,	left_num_queue:11,	Candidates:46 , Type:System.Boolean, #of Candies:1832
SN#:21751,	RT(min):28.122566,	IsCustom:False,	left_num_queue:10,	Candidates:46 , Type:System.Boolean, #of Candies:1832
SN#:21752,	RT(min):28.124924,	IsCustom:False,	left_num_queue:9,	Candidates:46 , Type:System.Boolean, #of Candies:1832
SN#:21753,	RT(min):28.127284,	IsCustom:False,	left_num_queue:8,	Candidates:46 , Type:System.Boolean, #of Candies:1832
SN#:21754,	RT(min):28.12966,	IsCustom:False,	left_num_queue:7,	Candidates:46 , Type:System.Boolean, #of Candies:1832
SN#:21755,	RT(min):28.13202,	IsCustom:False,	left_num_queue:6,	Candidates:47 , Type:System.Boolean, #of Candies:1832
SN#:21756,	RT(min):28.134378,	IsCustom:False,	left_num_queue:5,	Candidates:47 , Type:System.Boolean, #of Candies:1832
SN#:21757,	RT(min):28.139258,	IsCustom:False,	left_num_queue:4,	Candidates:47 , Type:System.Boolean, #of Candies:1832
SN#:21758,	RT(min):28.141599,	IsCustom:False,	left_num_queue:3,	Candidates:47 , Type:System.Boolean, #of Candies:1832
#MATCHED	28.143739	TASEFDSAIAQDK[HEAVYK]	0	0.997367130172324 FALSE 2444815 2025286.5,2444815,2286255.25,1895235.125,1347469.125,1445
SN#:21759,	RT(min):28.143739,	IsCustom:False,	left_num_queue:49,	Candidates:47 , Type:System.Boolean, #of Candies:1832
SN#:21760,	RT(min):28.145264,	IsCustom:False,	left_num_queue:48,	Candidates:47 , Type:System.Boolean, #of Candies:1832
SN#:21761,	RT(min):28.146807,	IsCustom:False,	left_num_queue:47,	Candidates:48 , Type:System.Boolean, #of Candies:1832
SN#:21762,	RT(min):28.147554,	IsCustom:False,	left_num_queue:47,	Candidates:48 , Type:System.Boolean, #of Candies:1832
SN#:21763,	RT(min):28.149856,	IsCustom:False,	left_num_queue:46,	Candidates:48 , Type:System.Boolean, #of Candies:1832
#STANDARD PEPTIDE WAS DETECTED	: SPGAPGLTLK[HEAVYK]	AT 28.151	AND 2 ANALYTES ARE UPDATED.	DPSOCRE=0.99990055018904, MISSEDNUM=1
SN#:21764,	RT(min):28.150714,	IsCustom:False,	left_num_queue:45,	Candidates:49 , Type:System.Boolean, #of Candies:1832
SN#:21765,	RT(min):28.151575,	IsCustom:False,	left_num_queue:44,	Candidates:49 , Type:System.Boolean, #of Candies:1832
SN#:21766,	RT(min):28.152341,	IsCustom:False,	left_num_queue:43,	Candidates:49 , Type:System.Boolean, #of Candies:1832
SN#:21767,	RT(min):28.1532,	IsCustom:False,	left_num_queue:42,	Candidates:49 , Type:System.Boolean, #of Candies:1832
SN#:21768,	RT(min):28.15406,	IsCustom:False,	left_num_queue:41,	Candidates:49 , Type:System.Boolean, #of Candies:1832
SN#:21769,	RT(min):28.154918,	IsCustom:False,	left_num_queue:40,	Candidates:49 , Type:System.Boolean, #of Candies:1832
SN#:21770,	RT(min):28.155779,	IsCustom:False,	left_num_queue:39,	Candidates:49 , Type:System.Boolean, #of Candies:1832
SN#:21771,	RT(min):28.156654,	IsCustom:False,	left_num_queue:38,	Candidates:49 , Type:System.Boolean, #of Candies:1832
SN#:21772,	RT(min):28.157512,	IsCustom:False,	left_num_queue:37,	Candidates:49 , Type:System.Boolean, #of Candies:1832
SN#:21773,	RT(min):28.158373,	IsCustom:False,	left_num_queue:36,	Candidates:49 , Type:System.Boolean, #of Candies:1832
#STANDARD PEPTIDE WAS DETECTED	: LTSDSTVYDYAGK[HEAVYK]	AT 28.159	AND 2 ANALYTES ARE UPDATED.	DPSOCRE=0.983364098238949, MISSEDNUM=0
SN#:21774,	RT(min):28.159237,	IsCustom:False,	left_num_queue:35,	Candidates:50 , Type:System.Boolean, #of Candies:1832
SN#:21775,	RT(min):28.160095,	IsCustom:False,	left_num_queue:34,	Candidates:50 , Type:System.Boolean, #of Candies:1832
SN#:21776,	RT(min):28.160954,	IsCustom:False,	left_num_queue:33,	Candidates:50 , Type:System.Boolean, #of Candies:1832
SN#:21777,	RT(min):28.161797,	IsCustom:False,	left_num_queue:32,	Candidates:50 , Type:System.Boolean, #of Candies:1832
SN#:21778,	RT(min):28.162656,	IsCustom:False,	left_num_queue:31,	Candidates:50 , Type:System.Boolean, #of Candies:1832
SN#:21779,	RT(min):28.163514,	IsCustom:False,	left_num_queue:30,	Candidates:50 , Type:System.Boolean, #of Candies:1832
SN#:21780,	RT(min):28.164391,	IsCustom:False,	left_num_queue:29,	Candidates:50 , Type:System.Boolean, #of Candies:1832
#STANDARD PEPTIDE WAS DETECTED	: IQAEVEAQLAR[HEAVYR]	AT 28.165	AND 2 ANALYTES ARE UPDATED.	DPSOCRE=0.992033046118994, MISSEDNUM=0
SN#:21781,	RT(min):28.165249,	IsCustom:False,	left_num_queue:28,	Candidates:51 , Type:System.Boolean, #of Candies:1832
SN#:21782,	RT(min):28.166125,	IsCustom:False,	left_num_queue:27,	Candidates:51 , Type:System.Boolean, #of Candies:1832
SN#:21783,	RT(min):28.166985,	IsCustom:False,	left_num_queue:26,	Candidates:51 , Type:System.Boolean, #of Candies:1832
SN#:21784,	RT(min):28.167826,	IsCustom:False,	left_num_queue:25,	Candidates:51 , Type:System.Boolean, #of Candies:1832